

UniCat Colloquium

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Computer-automated generation of microkinetic mechanisms

Microkinetic modeling is a powerful tool in predictive kinetics for heterogeneous catalysis. A major bottleneck in microkinetic modeling is the time required to compile the list of elementary reactions and ensure its thermodynamic consistency. I will present recent work on the software, RMG-Cat, that will automatically generate a microkinetic mechanism. The software is based upon similar software for gas-phase kinetics. The talk will discuss some of the challenges in porting the code from 3D (homogeneous) to 2D (heterogeneous) mechanism development. Preliminary results for CH₄ on Ni will be presented.

Wednesday, July 06, 2016 at 5:15 PM

TU Berlin, Institute of Chemistry
Straße des 17. Juni 115, 10623 Berlin

Building C, Lecture Hall **C 264**

Prof. Dr. Kraume (TUB)

Organizer

Coffee and cake will be served 30 minutes before the lecture. Guests are cordially invited to attend!
Prof. Dr. Matthias Driess - Chair of the Cluster of Excellence UniCat - www.unicat.tu-berlin.de



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